

# Superconducting ground state of the two-dimensional Hubbard model: a variational study

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## Abstract

A trial wave function is proposed for studying the instability of the two-dimensional Hubbard model with respect to  $d$ -wave superconductivity. Double occupancy is reduced in a similar way as in previous variational studies, but in addition our wave function both enhances the delocalization of holes and induces a kinetic exchange between the electron spins. These refinements lead to a large energy gain, while the pairing appears to be weakly affected by the additional term in the variational wave function.

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## 1. Introduction

The insulating antiferromagnetic phase of layered cuprates is well described by the two-dimensional Hubbard model at half filling. It is less clear whether this model is also able to describe the superconducting phase observed for hole concentrations  $0.25 < p < 0.5$ . It has been shown a long time ago that fermions with purely repulsive interactions can become superconducting, but the initial estimates for the critical temperature of continuum models were deceptively low [1]. In the mean-time, both analytical and numerical studies have indicated that for electrons on a lattice the situation may not be hopeless. Unfortunately, reliable estimates for the superconducting gap  $\Delta$ , the condensation energy  $W_n - W_s$  or other important quantities for the two-dimensional repulsive Hubbard model and variants thereof are still missing.

Here we report on the current status of our variational studies of the two-dimensional Hubbard model for intermediate values of  $U$  and a hole doping  $p \approx 0.19$ . Our preliminary results for the gap and the condensation energy are consistent with typical experimental values.

## 2. Variational approach

There are two competing terms in the Hubbard Hamiltonian  $\hat{H} = -t\hat{T} + U\hat{D}$ , the hopping term between nearest-neighbour sites

$$\hat{T} = \sum_{\langle i,j \rangle, \sigma} (c_{i\sigma}^\dagger c_{j\sigma} + c_{j\sigma}^\dagger c_{i\sigma}), \quad (1)$$

where  $c_{i\sigma}^\dagger$  creates an electron at site  $i$  with spin  $\sigma$ , and the on-site interaction (the number of doubly occupied sites)

$$\hat{D} = \sum_i n_{i\uparrow} n_{i\downarrow}, \quad n_{i\sigma} = c_{i\sigma}^\dagger c_{i\sigma}. \quad (2)$$

Several variational studies have been performed for the limiting case  $U \rightarrow \infty$ , where double occupancy is completely suppressed [2,3]. This limit is not appropriate for intermediate values of  $U$ . We have thus chosen the variational ansatz

$$|\Phi\rangle = e^{-h\hat{T}} e^{-g\hat{D}} |d\text{BCS}\rangle, \quad (3)$$

where double occupancy is only partially suppressed (variational parameter  $g$ ). At the same time both the delocalization of holes and kinetic exchange between spins are enhanced (parameter  $h$ ). The parent state

$|d\text{BCS}\rangle$  is a BCS state with parameters describing  $d$ -wave pairing, *i.e.*,

$$u_{\mathbf{k}}^2 = \frac{1}{2} \left(1 + \frac{\epsilon_{\mathbf{k}} - \mu}{E_{\mathbf{k}}}\right), \quad u_{\mathbf{k}} v_{\mathbf{k}} = \frac{\Delta_{\mathbf{k}}}{2E_{\mathbf{k}}}$$

with

$$E_{\mathbf{k}} = \sqrt{(\epsilon_{\mathbf{k}} - \mu)^2 + \Delta_{\mathbf{k}}^2}, \quad \Delta_{\mathbf{k}} = \Delta \cdot (\cos k_x - \cos k_y).$$

We notice that our wave function contains two additional variational parameters, the gap  $\Delta$  and the “chemical potential”  $\mu$  ( $\mu$  is a variational parameter and not the true chemical potential).

The expectation value of the Hamiltonian with respect to our trial state is computed using a Monte Carlo simulation. This is straightforward for  $h = 0$ , where the BCS state can be projected onto a subspace with a fixed number of particles and written as a superposition of real space configurations. For  $h > 0$  the projection onto a state with a fixed number of particles is found to lead to minus sign problems, which worsen as the gap parameter increases. The problem can be solved by using a fixed “chemical potential” (instead of a fixed number of particles) together with a momentum space representation. A Hubbard-Stratonovich transformation is used to decouple the on-site interaction in the Gutzwiller projector. Unfortunately, this approach results in a very slow convergence.

### 3. Results and conclusions

We have first considered the particular case  $h = 0$ , which has been studied previously [4]. Fig. 1 shows the energy per site as a function of the gap  $\Delta$  for several values of  $U$ . For  $U = 2t$  the numerical precision does not allow to draw any conclusion about pairing, but for  $U = 4t$  and  $U = 8t$  there are clear minima at  $\Delta \approx 0.04t$  and  $\Delta \approx 0.05t$ , respectively.

Allowing  $h$  to vary improves significantly both the energy and the wave function [5,6]. For  $U = 8t$ , the energy gain due to the refinement of the variational ansatz is two orders of magnitude larger than the condensation energy of Fig. 1. Nevertheless, our first results for  $h > 0$  confirm the trend towards  $d$ -wave superconductivity, with a gap of about the same size as in Fig. 1.

We briefly comment on the comparison between our results (for  $U = 8t$ ,  $t = 300$  meV and  $n = 1 - p \approx 0.81$ ) and experimental data for the layered cuprates. Typical data for the gap parameter found in photoemission experiments are  $\Delta \approx 10 - 15$  meV

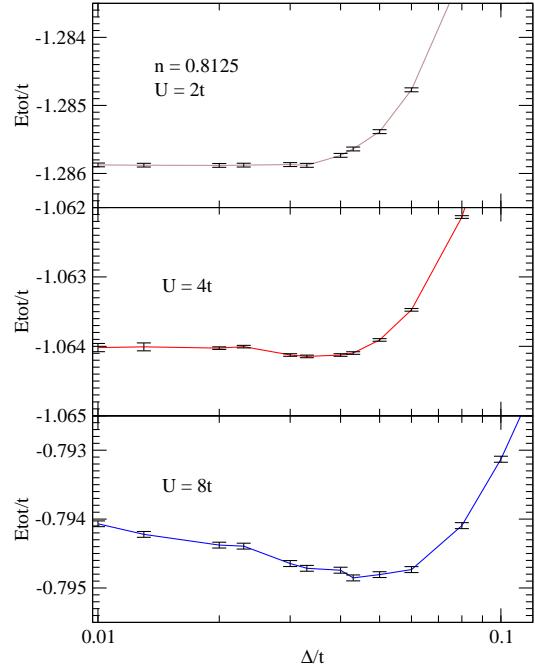


Fig. 1. Total energy per site of a 8x8 square lattice for a density corresponding to the slightly overdoped region of the phase diagram of cuprates.

[7], while the condensation energy obtained from specific heat data is of the order of 0.1 meV [8]. Both experimental values agree surprisingly well with our variational results.

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